

RESEARCH HIGHLIGHT

Basic Energy Sciences Program

Geosciences Subprogram

Title: Lattice-Gas Modeling of Retardation and Buoyancy in Fractures

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Objective: To test the effects of buoyancy and scaling on the extrapolation of dispersion and retardation coefficients from lab to field scale.

Results: Lattice-gas automata (LGA) were used to estimate errors in transport coefficients, as measured in laboratory experiments with Peclet numbers from 0 to 27.6 (defined relative to channel width), Damköhler numbers from 0.18 to ∞ , Grashof numbers of 0 or 75, and length/width up to 180. Low Damköhler numbers yield long, low-amplitude elution tails, which contain much of the total solute. As a consequence, at $Da \approx 0.18$ and $K_D = 8$, the solute *peak* travels at the same speed as the carrier fluid, yielding an *apparent* $K_D \approx 0$ after 5 characteristic diffusion times. Such conditions correspond (*e.g.*) to a meter-long path through a 0.5 cm-wide, gas-filled fracture. Buoyancy-enhanced dispersion, found in experiments with horizontal tubes, is confirmed by the LGA analysis (see Figure 1); however, a different mechanism is suggested for the enhancement in horizontal fractures. Both kinetic and buoyancy errors can be greatly reduced, or experiments made much smaller, if the first and second moments of a tracer pulse can be measured as functions of time.

Significance: Laboratory measurements are necessarily carried out in experiments that are very small compared to the flow paths and flow times expected in waste repositories and disposal sites. Care must be taken that the time scale of sorption in the experiment is small compared to the time scale of advection and diffusion through the system, or the effective retardation coefficients can be grossly underestimated, leading to unnecessarily conservative results in performance assessment. The problem is most serious when “core column tests” must be performed on a tight schedule, and has probably contributed to artificially low uranium retardation factors used for the analysis of at least one DOE site. LGA (and LB) analysis can help assure experiments are designed for proper extrapolation to the field distance and time scales.

Publication: “A Lattice-Gas Study of Retardation and Dispersion in Fractures: Assessment of Errors from Desorption Kinetics and Buoyancy”, by Harlan W. Stockman, accepted in *Water Resources Research*, 1997.

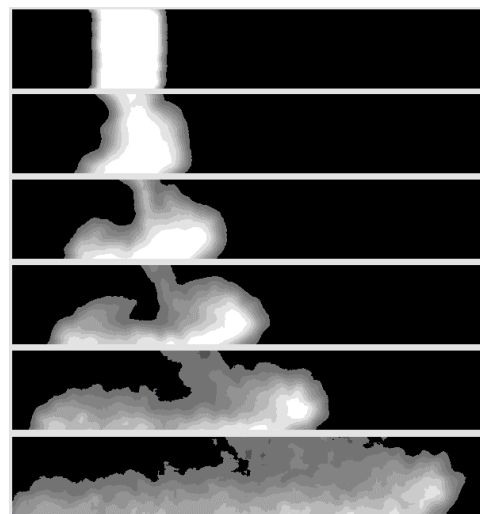


Figure 1. Six stages in the dispersion of a slug (white) that is initially $\approx 1\%$ denser than the carrier fluid (black). Flow is left to right; these frames show only $\approx 6\%$ of the entire channel length. The slug rapidly falls to the bottom of the channel, then disperses both forward and backward due to buoyancy-driven advection. Molecular diffusion gradually lessens the buoyancy contrast.